National Leadership Computing Facility

The National Leadership Computing Facility (NLCF), part of Oak Ridge National Laboratory's National Center for Computational Science, furnishes the computer, software, and expertise required by scientific communities for grand-challenge scale research.

The facility provides an unparalleled environment enabling new discoveries that will dramatically impact the nation's ability to produce a secure energy economy and increase mankind's understanding of our world, from the molecules in the air we breathe, to the birth and death of the stars in the sky.

Combustion simulation

The NLCF will make practical the first 3-D numerical simulations of an ignition flame fed by a fuel-air mix, with detailed chemistry. It will ultimately lead to more effective, predictive modeling that will help create much more fuel-efficient combustion devices. Simulation runs using the S3D software application can be completed in weeks, as opposed to months or years on other high-performance computing (HPC) systems.

Precise calculations of molecular structures

Chemists are using the NLCF systems and a new parallel-vector algorithm to perform precise calculations of molecular structures many times larger than were possible with other computer systems. Understanding these structures and establishing exact benchmarks are critically important for a wide range of pursuits, from studying contaminant dispersion in the environment to developing treatments for genetic diseases.

Plasma energy research

The NLCF resources run the world's fastest, most-detailed simulations of waves used to control plasma: gaseous matter superheated enough to generate massive amounts of energy. The simulation is related to the multibillion-dollar international ITER project, which aims to tame plasma so it can later become a virtually inexhaustible supply of 'clean' electricity. High-resolution simulations of the heated plasma take weeks, compared with years on other computer systems.

Accelerator design

Researchers will use NLCF supercomputers to help determine the optimal shape for the accelerator chamber inside the International Linear Collider (ILC). The ILC is the highest-priority future accelerator project in high-energy physics, and simulations are currently under way using the Omega3P code developed under the Department of Energy's SciDAC program.

Supernova research

The core collapse of a supernova—a massive star at the end of its life—creates a shock wave known as a stationary accretion shock instability (SASI) that may cause the star to explode. The

NLCF's computing power allows scientists to perform each 3-D SASI simulation in 1-2 days, compared with one month today, greatly speeding research.

Climate simulation

The NLCF will enable much greater fidelity and complexity in simulations of the global climate, providing more accurate predictions of climate change to inform major policy decisions. Increased resolution will resolve important dynamical processes in clouds and ocean eddies. New physical processes, such as enhanced atmospheric chemistry and a full carbon cycle, will not only increase accuracy but also open new avenues for scientific inquiry and prediction.

Nano-scale materials science

The NLCF resources and computational models are critical for nano-scale materials science, where the shortest relevant length scales are approaching the atomic limit and are therefore not straightforwardly accessible to experiment. Simulations of small metallic clusters are a key part of a research effort exploring an alternative future – engines powered by the combustion of tiny particles of metal.